

Partially scanned interferogram methodology applied to IASI for the retrieval of CO, CO₂, CH₄ and N₂O

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Abstract: The technique of partially scanned interferograms is applied to the retrieval of trace gases from Infrared Atmospheric Sounding Interferometer (IASI) observations. For the specific case of CO, CO₂, CH₄ and N₂O, we show that this methodology allows us to retrieve trace gases column abundances at an unprecedented accuracy at the level of the single IASI footprint. The technique consists in transforming the IASI spectra back to the interferogram domain where we identify small regions that are mostly sensitive to single gas species. The retrieval is then performed by directly applying Least Squares estimation to these small segments of interferometric radiances. One of the main advantages of the technique is that it allows the efficient use of the information contained in all the IASI channels that are available in the absorption bands of a specific gas species. The retrieval technique has been applied to IASI radiances measured over the Mediterranean sea during the month of July 2010, one of the hottest months on record. Results have been validated against ground-based measurements. We have also carried out a comparison with Atmospheric Infrared Radiometer Sounder data and IASI retrievals obtained with usual variational approaches in the spectral domain.

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1. Introduction

Fourier Transform Spectroscopy with Partially Scanned Interferograms (PSI) for the retrieval of trace gases from Infrared Atmospheric Sounding Interferometer (IASI [1]) observations has been recently investigated by [2–5]. PSI is used to compute the difference between spectra of atmospheric radiances at two different spectral resolutions. This differentiation of the spectrum acts as a high pass filter, which eliminates from the spectrum the low pass components, which include the surface emission in atmospheric window spectral regions. This property is particularly useful for nadir-looking instruments, where we need to separate the atmospheric windows emission component, which conveys information about atmospheric gases in the lower troposphere, from the surface emission.

PSI was first introduced by [6] for the retrieval of atmospheric parameters. Later on, [7] proposed a correlation interferometer for the observation of atmospheric trace gases, whereas

[8] further analysed and applied the PSI methodology to the direct inversion of small segments of interferometric radiances for the purpose of temperature retrieval.

When we apply PSI to the retrieval of total column amounts of trace gas species we exploit what is known as the multiplex or Fellgett gain of Fourier transform spectrometers. Each single interferogram sample is a linear combination of the entire set of spectral radiances forming the original spectrum. The peak contribution to top of atmosphere radiances comes from altitudes that change with wave number. Consequently, in the spectral domain we need to sample a relatively large portion of the spectrum if we want to retrieve information for an atmospheric column ranging from the Earth's surface to the top of the atmosphere. Conversely, because in the interferogram domain each data point conveys information from any region of the spectrum, the vertical portion of the atmospheric column covered by any individual interferogram sample is much larger than the portion covered by any spectral sample at a given wave number. In addition, the IASI spectral sampling of 0.25 cm^{-1} allows us to resolve the specific periodic patterns that characterize the spectra of linear molecules such as CO_2 , CO and N_2O . Due to the properties of the Fourier transform, these periodic patterns in the spectra result in well defined sharp signatures in the interferogram. This means that a small interval of the interferogram domain contains most of the information contained in the whole radiance spectrum. For instance, CO_2 absorption lines are typically characterized by a regular spacing of $\approx 0.8\text{ cm}^{-1}$, this results in a sharp resonance feature in the interferogram. The resonance can be found at an optical path difference equal to the inverse of two times the spacing, i.e. $\approx 0.63\text{ cm}$.

Following the PSI approach, [3–5] developed an estimation statistical method, which is based on a polynomial regression between interferogram radiance and the total column amount (TCA) of the trace gas. This *parametric* approach is computationally fast because does not require the calculation of Jacobian derivatives and allowed us to achieve accuracies, at the level of the single IASI observation (which has a footprint of 12 km radius at nadir), of about $\pm 9\text{ ppmv}$ for CO_2 , $\approx \pm 16\text{ ppbv}$ for CO , $\approx \pm 0.1\text{ ppmv}$ for CH_4 and $\approx \pm 30\text{ ppbv}$ for N_2O [3, 5].

In this paper we show that the introduction of the use of Jacobian derivatives allows us to utilize a *non-parametric* approach where the radiative transfer equation is directly inverted through a conventional Least Squares estimation. Using this procedure we can achieve an estimate where the final accuracy has been improved by a factor between 3 and 10, depending on the molecule. The fast computation of the Jacobian derivatives has been made possible by improvements to our forward model for IASI, hereafter referred to as σ -IASI [9, 10]. These improvements have allowed us to run the code 100 times faster than the previous version.

The limb-sounding of upper and lower stratosphere trace species is amongst the main goals of many satellite missions, e.g. Atmospheric Chemistry Experiment [11], MIPAS (Michelson Interferometer for Passive Atmospheric Sounding) of the European Space Agency [12]. The objective of this study is to apply our methodology to the retrieval of trace gases from IASI, which is a nadir-looking instrument, with improved accuracy and horizontal spatial resolution.

The subject of remote sensing of atmospheric minor and trace gases from nadir looking instruments on board polar satellites is not a new subject. The sensors used for this scope include the Japanese IMG (Interferometric Monitoring of Greenhouse Gases) [13], the American AIRS (Atmospheric Infrared Radiometer Sounder) [14–16], the European IASI [3, 17–24] and the Japanese GOSAT (Greenhouse Gases Observing Satellite) [25].

In this paper we offer a different perspective focusing on the use of the PSI methodology and documenting its capability of achieving columnar contents of trace gases with an unprecedented accuracy. The PSI methodology has been applied to IASI data recorded during July 2010 over the Mediterranean sea. The July 2010 period has been selected because of the weather pattern over the Mediterranean, which has been characterized by above normal surface temperatures associated to a relatively high frequency of blocking days. Likewise, a particularly long block-

ing event has been experienced over Western Russia that has led to the occurrence of anomalously high temperatures over this region. Thus, we have decided to use our methodology to investigate whether the quiescent weather and the high temperatures could have resulted in any detectable behaviour in the concentration of the trace gases considered in this paper.

The state vector (surface temperature, temperature, H₂O and O₃ atmospheric profiles), which is needed to initialize the estimation procedure for the total column amount of trace gases, has been retrieved directly from IASI radiances, through the forward/inverse package that we call φ -IASI. The mathematical aspects and validation of φ -IASI have been discussed in detail in various publications [9, 10, 26–32]. Ancillary information used to constrain the retrieval of the atmospheric state vector has been obtained from the European Centre for Medium range Weather Forecasts (ECMWF) analyses, collocated in time and space with the IASI soundings.

The paper is organized as follows. In section 2 we describe the IASI data and the new aspects of our forward model σ -IASI, whereas the description of the basic methods used in the PSI approach is presented in sections 3. The retrieval methodology for CO₂, CO, CH₄ and N₂O is discussed in sections 3.1 and 3.2. Section 3.1 covers the case of CO₂ and is mainly intended to give an example of the overall retrieval methodology. Results obtained from the use of IASI data are presented for the aforementioned Mediterranean basin case study in section 4, where we also show a comparison to AIRS data and IASI retrievals obtained with variational approaches in the spectral domain [23, 24]. Finally, conclusions are drawn in section 5.

2. Data

IASI observations used in this work have been recorded during the entire month of July 2010 over the Mediterranean sea. We concentrate on clear sky, sea surface soundings. However, the retrieval methodology can be applied to any kind of surface.

IASI, which is flying on board the Metop-A/B (Meteorological Operational Satellite) platforms, has been developed in France by the Centre National d'Etudes Spatiales (CNES) and is the first of three satellites of the European Organization for the Exploitation of Meteorological Satellites (EUMETSAT) European Polar System (EPS). The IASI instrument [1] covers the spectral range from 645 to 2760 cm⁻¹ (3.62 to 15.50 μ m), with a sampling interval $\Delta\sigma = 0.25$ cm⁻¹. Thus, each single spectrum is formed by 8461 data points or channels. The calibrated IASI interferogram extends from 0 to a maximum optical path difference of 2 cm. IASI is an across track scanning system with a swath range of $\pm 48^\circ 20'$. The scan movement is symmetric with respect to the nadir direction and results in a scan line with thirty footprint positions on the Earth's surface. The effective field of view (EFOV) is the useful field of view at each scan position or footprint. Each footprint consists of a 2×2 matrix of instantaneous fields of view (IFOV). Any single IFOV has a diameter of 14.65 mrad, which corresponds to a ground resolution of 12 km at nadir assuming a satellite altitude of 819 km. The 2×2 matrix is centred on the viewing direction.

The IASI spectra were screened for cloud contamination using the IASI stand alone cloud detection algorithm developed by the authors [28–31]. After cloud detection, a total of 34719 IASI spectra were selected.

For comparison purposes we have utilized AIRS level 2 CO₂ products (AIRS version 5) for the same area and dates [33]. The data are not gridded and their horizontal spatial resolution is 90 km, which is coarser than the IASI 12 km resolution. For the case of CO, we have also used IASI data utilizing a different retrieval scheme. This is the scheme developed at LATMOS-ULB (Laboratoire d'Optique Atmosphérique - Université libre de Bruxelles) [23, 24]. LATMOS-ULB IASI Level 2 CO data for the whole month of July 2010 over the Mediterranean basin have been downloaded from the Atmospheric Chemistry Data Center [34] site.

Sea level July averages of CO₂, CH₄ and N₂O concentrations obtained from a number of

Global Atmosphere Watch (GAW) (World Meteorological Organization) WMO stations located in the Mediterranean basin have been also used.

To specify the water vapour and ozone background vectors and covariance matrices utilized in the inversion of the IASI spectra, we have used ECMWF atmospheric analysis fields at 00:00, 06:00, 12:00 and 18:00 UTC during July 2010. The version of the ECMWF model which was operational at that time was characterized by a vertical discretization of the atmosphere into 91 pressure levels with the model top at 0.01 hPa and a horizontal truncation of T1279. This truncation corresponds to a grid spacing of about 16km or, equivalently, to a horizontal grid box of $0.141^\circ \times 0.141^\circ$. The vertical coordinates of the model are surfaces of constant pressure in the upper stratosphere and lower mesosphere whereas they follow the earth's surface in the lower and mid-troposphere. In terms of vertical resolution (measured in geometric height), this is highest in the planetary boundary and lowest in the stratosphere and lower mesosphere. The analysis fields were extracted from the ECMWF archive at the full T1279 resolution, interpolated to a grid of points with a separation of $0.3^\circ \times 0.3^\circ$ and then collocated in both space and time to the IASI soundings used in this study.

For T (temperature profile) and T_s (surface temperature) our IASI retrieval algorithm does not use the ECMWF analyses. These two parameters are first directly estimated from IASI observations with an Empirical Orthogonal Function linear regression procedure and, finally, simultaneously retrieved with the other parameters through iterations with a physical inverse scheme. This final physical retrieval step retrieves simultaneously the state vector $(T, Q, O, T_s, \varepsilon)$, where Q is the water vapour mixing ratio profile (units of g/kg), O is the ozone mixing ratio profile (units of ppmv) and ε the surface emissivity spectrum. The most recent version of the scheme can be found in [32]. Trace gases are not retrieved at this stage, their retrieval is performed sequentially using the PSI scheme utilizing the state vector $(T, Q, O, T_s, \varepsilon)$ previously estimated from IASI.

2.1. Forward model

Radiative transfer calculations are based on our σ -IASI model [9]. The σ -IASI package consists of a monochromatic radiative transfer computer code designed for the fast computation of spectral radiances and their derivatives (Jacobians) with respect to a set of geophysical parameters. In its original formulation σ -IASI uses a vertical grid of sixty atmospheric layers bounded by pressure levels ranging from 1050 to 0.005 hPa. The model is based on a look-up table of optical depths computed using the line-by-line code LBLRTM [35]. The current optical depth look-up table is based on LBLRTM version 12 released on January 2011 in conjunction with the water vapour continuum model MT_CKD version 2.5.2 and the line file aer_v3.0 [36]. The σ -IASI model parameterizes the monochromatic optical depths using a second order polynomial. At a given pressure, the optical depth for the generic i -th molecule, is computed according to

$$\chi_{\sigma,i} = q_i (c_{\sigma,0,i} + c_{\sigma,1,i}T + c_{\sigma,2,i}T^2) \quad (1)$$

where T is the temperature, q_i the molecule concentration and $c_{\sigma,j,i}$ with $j = 0, 1, 2$, are the regression coefficients which are obtained using a Least Squares procedure and are themselves stored in the optical depth look-up-table. For water vapour, unlike other gases, in order to take into account effects depending on the gas concentration, such as self-broadening, a bi-dimensional look-up-table is used [37]. Thus, for water vapour, identified with $i = 1$, the optical depths is calculated according to

$$\chi_{\sigma,1} = q_1 (c_{\sigma,0,1} + c_{\sigma,1,1}T + c_{\sigma,2,1}T^2 + c_{\sigma,3,1}q_1) \quad (2)$$

The subscript σ indicates the monochromatic quantities. In the original version of σ -IASI [9], the monochromatic optical depth was computed and parameterized at the spectral resolution of

10^{-4} cm^{-1} . A recent analysis of the trade-off between accuracy and computational efficiency of the code has shown that this spectral sampling can be reduced without sacrificing the robustness and accuracy of the inverse scheme. The analysis has shown that for IASI, the optical depth can be averaged and re-sampled at the lower rate of 10^{-2} cm^{-1} . This is referred to as lut-coarse (look-up-table-coarse) sampling in contrast to the lut-fine sampling of 10^{-4} cm^{-1} . Also, in the case of the lut-coarse sampling interval, the optical depth can be parameterized with a low order polynomial where the regression coefficients are obtained as explained below. For each species i we can define an equivalent optical depth $\chi_{\langle\sigma\rangle,i}$, which can be parameterized with respect to temperature in the same way we do for lut-fine sampled quantities (Eqs. (1) and (2)). The equivalent optical depth is

$$\chi_{\langle\sigma\rangle,i} = q_i (c_{\langle\sigma\rangle,0,i} + c_{\langle\sigma\rangle,1,i}T + c_{\langle\sigma\rangle,2,i}T^2) \quad (3)$$

where the angular brackets, $\langle \cdot \rangle$ indicates the average operation over the wave number. In Eq. (3) the equivalent coefficients $c_{\langle\sigma\rangle,j,i}$ with $j = 0, 1, 2$, are obtained by fitting the layer transmittance averaged from the fine to the coarse spectral resolution

$$q_i (c_{\langle\sigma\rangle,0,i} + c_{\langle\sigma\rangle,1,i}T + c_{\langle\sigma\rangle,2,i}T^2) = -\log(\langle \tau_{\sigma,i} \rangle) = -\log[\langle \exp(-\chi_{\sigma,i}) \rangle] \quad (4)$$

Due to the lut-coarse sampling and other optimizations, σ -IASI runs more than 100 times faster than the older version that used the fine-mesh look-up table. It is also to be stressed that the code with the lut-coarse sampling may not be appropriate for use in the upper stratosphere where the representation of the features of the CO_2 absorption would be as a result significantly degraded. The lut-coarse sampling does not affect, however, the results presented in this paper where we are mainly interested in the study of the lower atmosphere.

3. PSI basics and retrieval methodology

For a Fourier transform spectrometer such as IASI the quantity which is effectively measured is the interferogram, $I(x)$, with x the OPD (optical path difference in units of cm). The spectrum, $R(\sigma)$, with σ the wave number (in units of cm^{-1}) is recovered through a Fourier transform operation. For a calibrated, bandlimited spectrum, whatever its origin and measurement technique, the interferogram is simply computed as the Fourier transform of the symmetrized spectrum, $r(\sigma)$

$$I(x) = \int_{-\infty}^{+\infty} r(\sigma) \exp(2\pi i \sigma x) d\sigma; \quad \text{with} \quad r(\pm\sigma) = \begin{cases} \frac{R(\sigma)}{2}; & \sigma_1 < \sigma < \sigma_2 \\ 0; & \text{otherwise} \end{cases} \quad (5)$$

with i the imaginary unit and σ_1, σ_2 are the band endpoints. The bandwidth is $\sigma_2 - \sigma_1$ and both endpoints are positive. In this way, the interferogram can be thought of as a mathematical tool which can be applied to any kind of spectrum, either measured with a radiometer or an interferometer. A partial interferogram, $I(x); x_1 \leq x \leq x_2$, is the interferogram over a given optical path difference interval with endpoints, x_1 and x_2 , respectively. Details about the properties of the partial interferogram can be found in [3]. For the present analysis, these properties are well illustrated by the case for CO_2 whose periodic pattern of absorption lines, superimposed on vibrational transitions, yields a typical interferogram resonance around $x = 0.65 \text{ cm}$. This resonance is plotted in Fig. 1, which shows a typical interferogram for a tropical IASI sounding. The interferogram has been obtained by considering the IASI band 1 (645 to 1210 cm^{-1}) alone. In this band we have the ν_2 fundamental absorption band of CO_2 and the hot bands in the atmospheric window. It is important to stress that the partial interferogram shown in Fig. 1 conveys information from the entire IASI band 1. This means that due to the spectral characteristics of CO_2 lines, all the IASI band 1 information on CO_2 emission is compressed in a relatively

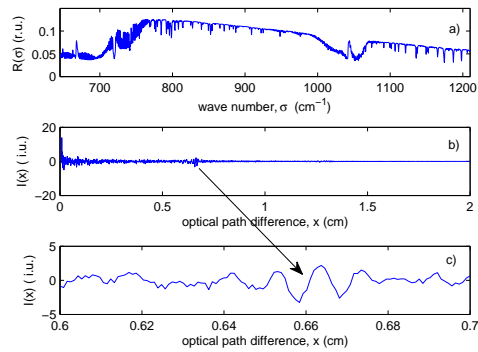


Fig. 1. a) IASI band 1 spectrum for a tropical sounding; b) its interferogram; c) partial interferogram over the range 0.6-0.7 cm, which evidences the beating due to the CO₂ line emission structure. The spectrum is in radiance units (1 r.u.=1 W m⁻² sr⁻¹ (cm⁻¹)⁻¹); the interferogram is in interferogram units (1 i.u.= 1 W m⁻² sr⁻¹).

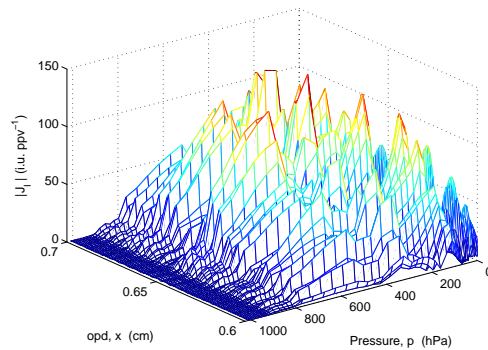


Fig. 2. Mesh surface of J_I : the Jacobian derivative of the interferogram radiance with respect to mixing ratio profile of CO₂ (1 i.u.= 1 W m⁻² sr⁻¹).

small interval in the interferogram domain. This is all the more evident when we consider the sensitivity of the partial interferogram to the concentration of CO₂. The sensitivity is computed as the Jacobian derivative of the interferogram radiance, J_I with respect to the CO₂ atmospheric profile, that is

$$J_I(x, p) = \frac{\partial I(x)}{\partial q_{CO_2}(p)} \quad (6)$$

where $q_{CO_2}(p)$ (with p the pressure) is the mixing ratio profile of CO₂. The Jacobian derivative is shown in the mesh surface of Fig. 2 for the range of OPD around the CO₂ resonance. From this figure we see that the sensitivity of $I(x)$ to CO₂ extends throughout the entire atmospheric column, down below to the planetary boundary layer.

3.1. The case of CO₂

For the retrieval of the total column amount of CO₂, we consider the partial interferogram which extends from $x_1 = 0.55$ cm to $x_2 = 0.75$ cm. This interferogram is derived from IASI

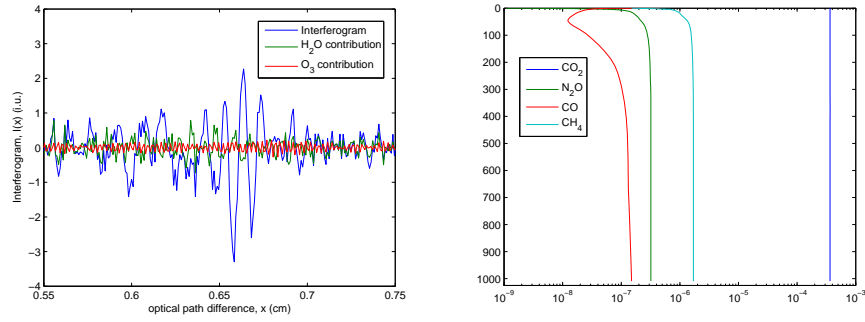


Fig. 3. (left) Exemplifying the partial interferogram used for the retrieval of CO₂. The figure also shows the signal contributed from two possible interfering atmospheric gases (1 i.u.= 1 W m⁻²sr⁻¹). (right) Reference mixing ratio profiles for the trace gases analyzed in this paper.

radiances in band 1, which covers the range from 645 to 1210 cm⁻¹. The partial interferogram is shown in Fig. 3 for the case of a typical tropical air mass. The contribution to the signal due to the potential interfering molecules H₂O and O₃ is also shown in the figure. For the generic interfering factor, X , the contribution to the interferogram is computed by considering the difference, $I(x) - I_X(x)$, where $I(x)$ is the interferogram with the *full* state vector, and $I_X(x)$ that with the state vector where X has been set to zero. It is seen that within the range 0.55-0.75 cm the interferogram signal is mostly due to CO₂. The effect of H₂O is significant, whereas that of O₃ can be considered to be an effect of second order.

For the specific case of IASI, the number of interferogram samples within the range 0.55-0.75 cm is $N = 227$. Let \mathbf{I} be the interferogram vector, $\mathbf{I} = (I_1, \dots, I_N)^T$, where the super-script T stands for transpose and I_j stands for $I(x_j)$, $j = 1, \dots, N$ and let $\mathbf{v} = (\mathbf{q}_{CO_2}, \mathbf{T}, \mathbf{Q}, T_s)^T$ be the state vector. We develop the interferogram in a Taylor series around a reference state vector, \mathbf{v}_o truncated at the first order term,

$$\mathbf{I} = \mathbf{I}_o + \mathbf{J}_{CO_2}(\mathbf{q}_{CO_2} - \mathbf{q}_{CO_2,o}) + \mathbf{J}_T(\mathbf{T} - \mathbf{T}_o) + \mathbf{J}_Q(\mathbf{Q} - \mathbf{Q}_o) + \mathbf{J}_s(T_s - T_{s,o}) \quad (7)$$

where, as usual, as before T_s is the surface temperature, \mathbf{T} the temperature profile, \mathbf{Q} the water vapour profile and \mathbf{q}_{CO_2} the CO₂ profile. The reference state vector, \mathbf{v}_o , apart from the CO₂ profile, is that determined by physical inversion of the same IASI spectrum as that we use for the final retrieval of CO₂. The Jacobian derivatives are computed as usual at the reference state vector.

Because the reference atmospheric state \mathbf{v}_o has been itself retrieved by using IASI observations, the assumption of linearity is reasonable, unless the retrieval failed. In addition, we do not need at this stage to retrieve the fine structures of the vertical profiles of T and Q . These parameters are included, along with T_s , to avoid that their residual uncertainty could bias the final estimate of the total column amount of CO₂. For this reason we assume that the true and the reference atmospheric parameters may be different up to a scaling factor, that is

$$\begin{aligned} T_s &= (1 + f_{T_s})T_{s,o}; & \mathbf{T} &= (1 + f_T)\mathbf{T}_o \\ \mathbf{Q} &= (1 + f_Q)\mathbf{Q}_o; & \mathbf{q}_{CO_2} &= (1 + f_{CO_2})\mathbf{q}_{CO_2,o} \end{aligned} \quad (8)$$

With this assumption, Eq. (7) simplifies in

$$\begin{aligned} \mathbf{I} - \mathbf{I}_o &= \mathbf{a}_1 f_{CO_2} + \mathbf{a}_2 f_T + \mathbf{a}_3 f_Q + \mathbf{a}_4 f_{T_s} \\ \mathbf{a}_1 &= \mathbf{J}_{CO_2} \mathbf{q}_{CO_2,o}; & \mathbf{a}_2 &= \mathbf{J}_T \mathbf{T}_o; & \mathbf{a}_3 &= \mathbf{J}_Q \mathbf{Q}_o; & \mathbf{a}_4 &= \mathbf{J}_s T_{s,o} \end{aligned} \quad (9)$$